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Amendments to the Specification:

On page 4, please replace lines 10-26 with the following:

DESCRIPTION OF THE SPECIFIC EMBODIMENTS

The computer molecular modeling may be self-validated in accordance with the present invention. Molecule modeling and simulations are made with certain approximations, such as rigid body approximations of clusters of atoms, and the parameters of the models of the force fields, solvents, initial conditions, and other environmental and internal models. Though the present invention is not necessarily limited to such molecular modeling and simulations as described in co-pending U.S. Patent Application No. 1] 10/053,253, entitled "Method for Large Timesteps in Molecular Modeling" and claiming priority to the above-referenced Provisional Patent Application No. 60/245,688; U.S. Patent Application No. [] 10/053,354, entitled "Method for Residual Form in Molecular Modeling" [["]] and claiming priority to the above-referenced Provisional Patent Application No. 60/245,731; and U.S. Patent Application No. [[]] 10/053,348, entitled [[""]] "Method for Analytical Jacobian Computation in Molecular Modeling" and claiming priority to the above-referenced Provisional Patent Application No. 60/245,730; all of which patent applications filed of even date, assigned to the present assignee and incorporated by reference in their entirety, the resulting high-speed molecular modeling taught therein are particularly useful in exploiting the advantages of the present invention.